

The role of boson-fermion correlations in the resonance theory of superfluids

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Correlations between a composite boson and a fermion pair are considered in the context of the crossover theory of fermionic to bosonic superfluidity. It is shown that such correlations are the minimal ingredients needed in a many-body theory to generate the right boson-boson scattering length in the Bose-Einstein limit of the crossover.

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In the quantum theory of many-body systems, superfluidity is connected with a broken symmetry which is not anticipated from the underlying microscopic Hamiltonian. There are two distinct types of superfluidity. A first type occurs in fermionic systems in the presence of an effectively attractive fermion-fermion interaction (as in superconducting metals). The symmetry breaking there is associated with the development of mean-field pair-correlations with coherence length much larger than the interparticle spacing. A second type of superfluidity occurs in bosonic systems (such as atomic condensates) where the symmetry breaking is associated with the condensation of preformed bosons with spatial size much smaller than the interparticle spacing. For many years it has been conjectured that these two types of superfluidity are in fact alternative limits of a single universal phenomenon, and that one could continuously pass from fermionic to bosonic superfluidity by properly varying the fermion interaction parameters.

This conjecture has attracted a great deal of attention. It has been shown that the Bardeen-Cooper-Schrieffer (BCS) theory [1] reduces to Bose-Einstein condensation (BEC) of bosonic dimers as the pair correlation length becomes small compared with the interparticle spacing [2]. For a dilute Fermi gas, in which the mean interparticle spacing is large compared to the extension of the two-body potential, the simplest way to obtain the crossover is via a scattering resonance. This corresponds to bringing the highest-lying bound state from just above to just below threshold. In a dilute gas the atom-atom interaction can be parametrized by the only nonvanishing contribution to the two-body T -matrix at low energy, namely the fermionic s -wave scattering length a_F (with $T = 4\pi\hbar^2 a_F/m$ and m is the atomic mass). The crossover from fermionic to bosonic superfluidity thus appears through the tuning of a_F from negative values, through infinity, to positive values. A series of improvements to the basic theory to better account for the crossover region have been developed and extensively studied during the last decades [3].

It has recently been pointed out [4, 5] that although these theories model the passage from fermionic to bosonic superfluidity, they have one major flaw in that they fail to reproduce the correct equation of state of the

system in the bosonic limit. This is due to the fact that they predict the wrong value for the boson-boson scattering length, $a_B = 2a_F$. A solution of the four-fermion Schrödinger equation for contact scattering in vacuum, which in principle can be determined exactly, has recently been found [5] and provided the value $a_B \simeq 0.6a_F$.

Progress in experiments with quantum atomic gases has lead to experimentally accessible systems which can directly address the crossover region using Feshbach scattering resonances [6]. Bose-Einstein condensation of two-fermion dimers has been observed and the experimental study of the crossover is actively being pursued. The first data collected on the Bose-Einstein condensed cloud were consistent with the $0.6a_F$ [7]. A consequence is that crossover theories that predict in the BEC limit the value $2a_F$ for the boson-boson scattering length will not yield the correct results for all observables dependent on interactions, e.g. the collective modes, the vortex core structure, the internal energy, and even the macroscopic spatial extent of a confined cloud.

The aim of this paper is to present a theory of the crossover which correctly reproduces the Gross-Pitaevskii and Bogoliubov theory of the non-ideal Bose gas with the right boson-boson interaction. As we shall see this theory will recover on the fermionic side the BCS theory including the Gorkov corrections due to density and spin fluctuations [8]. We begin by pointing out the essential ingredients which are missing in standard crossover theories and which have to be included to achieve this goal. Our approach was motivated by Ref. [5] where the few-body problem of four fermions interacting in vacuum was considered. The essential property leading to the correct boson-boson T -matrix was identified within the contact scattering formalism as the three-particle correlation between a composite boson and a fermion pair. This followed from the observation that in the limit in which the distance \mathbf{r}_1 between any two of the fermions becomes small, the four-fermion wavefunction must factorize as

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{R}) \rightarrow f(\mathbf{r}_2, \mathbf{R})(1/4\pi r_1 - 1/4\pi a_F), \quad (1)$$

where \mathbf{r}_2 is the distance between the two other fermions and $\mathbf{R}/\sqrt{2}$ the distance between the centers of mass of the pairs. The function $f(\mathbf{r}_2, \mathbf{R})$ —an effective three-body wavefunction of a composite boson and two fermions—

contains all information needed to determine the boson-boson scattering length. The reason why standard crossover theories fail to give the correct T -matrix in the BEC limit is then revealed, because they are typically based on the BCS assumption that only two-fermion correlations are important, and only those are withheld in the correlation hierarchy.

In this paper we show that a self-consistent many-body theory of the crossover can be constructed which includes three-particle correlations, and correctly reduces to the known results in the appropriate limits. This modification not only brings about quantitative corrections, but also introduces a qualitative change in the crossover picture. A major consequence is that the superfluid order parameter in this crossover theory is not given by the simple integration of a BCS-type pairing field.

A system of fermions in two internal states (\uparrow and \downarrow) close to a Feshbach resonance can be described using the many-body Hamiltonian [9, 10]:

$$\begin{aligned} \hat{H}_{\text{res}} = & \sum_{\mathbf{k}, \sigma=\uparrow, \downarrow} \epsilon_{\mathbf{k}} \hat{a}_{\mathbf{k}\sigma}^\dagger \hat{a}_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \left(\frac{\epsilon_{\mathbf{q}}}{2} + \nu \right) \hat{b}_{\mathbf{q}}^\dagger \hat{b}_{\mathbf{q}} \\ & + \sum_{\mathbf{q}, \mathbf{k}} g_{\mathbf{k}} \left(\hat{b}_{\mathbf{q}}^\dagger \hat{a}_{\mathbf{q}/2-\mathbf{k}\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}\uparrow} + \text{H.c.} \right) \end{aligned} \quad (2)$$

where $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ is the free fermion dispersion relation, $g_{\mathbf{k}}$ is the matrix element relating two free fermions in the open channel to the closed channel bound state near threshold, and ν is the bare detuning of the bound state. The operators $\hat{a}_{\mathbf{k}\sigma}^{(\dagger)}$ annihilate (create) open channel fermions with momentum \mathbf{k} and spin σ , while $\hat{b}_{\mathbf{k}}^{(\dagger)}$ annihilate (create) closed channel bosons. We ignore here the direct interaction of the fermionic degrees of freedom which would otherwise give rise to an asymptotic background value for the scattering length, since that plays no role at detunings sufficiently close to the resonance value. This can nevertheless be reintroduced in a straightforward manner as has been previously discussed [11].

In resonance superfluidity theory the information contained in the wavefunction $f(\mathbf{r}_2, \mathbf{R})$ for a boson and a fermion pair is in principle conveyed by the correlation function

$$\langle \hat{b}_{-\mathbf{q}} \hat{a}_{\mathbf{q}/2-\mathbf{k}\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}\uparrow} \rangle. \quad (3)$$

Notice, however, that the two quantities do not simply coincide because the one in Eq. (3) describes the correlations between bare fermionic and bosonic states, while $f(\mathbf{r}_2, \mathbf{R})$ gives the correlations between states dressed by the interactions (and thus physically observable). The connection between the two quantities is not obvious and must be stated explicitly.

The relation can be well understood by considering the two-fermion correlations with zero center of mass momentum, which in a vacuum coincides with the Fourier

transform of the relative wavefunction. The bare correlation function is simply $\langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle$. This can however never be an eigenstate of Eq. (2). An eigenstate can be constructed by considering the following linear combination of $\langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle$ and $\langle \hat{b}_0 \rangle$ (dressed state):

$$\Psi_{\mathbf{k}} = \langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle + \mathcal{P} \frac{g_{\mathbf{k}}}{2\epsilon_{\mathbf{k}} - E} \langle \hat{b}_0 \rangle \quad (4)$$

with \mathcal{P} denoting the Cauchy Principal Value and E a solution of

$$E = \nu - \mathcal{P} \sum_{\mathbf{k}} \frac{g_{\mathbf{k}}^2}{2\epsilon_{\mathbf{k}} - E}. \quad (5)$$

The nature of the solution depends on the presence or absence of a bound state indicated by the sign of the renormalized detuning $\bar{\nu}$. This is defined as

$$\bar{\nu} = \nu - \sum_{\mathbf{k}} \frac{g_{\mathbf{k}}^2}{2\epsilon_{\mathbf{k}}} \quad (6)$$

and is physically related to the magnetic field shift from the Feshbach resonance [11]. The case of $\bar{\nu} < 0$ corresponds to the BEC side of the resonance. There a bosonic dimer bound state exists and the solution of Eq. (5) coincides with the bound state energy $E = -\hbar^2 / ma_F^2$ [12, 13, 14]. For $\bar{\nu} > 0$ there is no bound state and the solution is $E = \bar{\nu}$. Evolving Eq. (4) for two particles in a vacuum under the Hamiltonian Eq. (2) gives the Schrödinger equation

$$i\hbar \frac{d\Psi_{\mathbf{k}}}{dt} = 2\epsilon_{\mathbf{k}} \Psi_{\mathbf{k}} + \sum_{\mathbf{k}'} U_{\mathbf{k}, \mathbf{k}'} \Psi_{\mathbf{k}'} \quad (7)$$

with real separable potential

$$U_{\mathbf{k}, \mathbf{k}'} = \mathcal{P} \frac{g_{\mathbf{k}} g_{\mathbf{k}'}}{2\epsilon_{\mathbf{k}} - E}. \quad (8)$$

What remains is to show that this potential generates the correct scattering length at all detunings $\bar{\nu}$. To this end we must obtain the T -matrix by solving the Lippmann-Schwinger equation as derived from Eq. (7) [15]

$$T_{\mathbf{k}, \mathbf{k}'} = U_{\mathbf{k}, \mathbf{k}'} + \sum_{\mathbf{q}} \frac{U_{\mathbf{k}, \mathbf{q}} T_{\mathbf{q}, \mathbf{k}'}}{2\epsilon_{\mathbf{k}'} - 2\epsilon_{\mathbf{q}} + i\delta}, \quad \delta \rightarrow 0^+ \quad (9)$$

in the limit of zero scattering energy. Substituting Eq. (8) into Eq. (9) and performing the integration, we recover the desired result for the zero-energy T -matrix

$$T = -\frac{g_0^2}{\bar{\nu}}. \quad (10)$$

Eq (10) provides the correct behavior of the tuning of the scattering length around resonance [11], with the usual definition $T = 4\pi\hbar^2 a_F / m$, and confirms that the potential in Eq. (8) leads to the correct effective fermion interaction properties.

The key point is that Eq. (7) is also the time-dependent Schrödinger equation for the relative wavefunction $\langle \hat{\alpha}_{-\mathbf{k}\downarrow} \hat{\alpha}_{\mathbf{k}\uparrow} \rangle$ of two particles in a vacuum evolving under the single-channel Hamiltonian

$$\begin{aligned} \hat{H}_{\text{single}} &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}\sigma}^\dagger \hat{\alpha}_{\mathbf{k}\sigma} \\ &+ \sum_{\mathbf{q}\mathbf{k}\mathbf{k}'} U_{\mathbf{k},\mathbf{k}'} \hat{\alpha}_{\mathbf{q}/2+\mathbf{k}\uparrow}^\dagger \hat{\alpha}_{\mathbf{q}/2-\mathbf{k}\downarrow}^\dagger \hat{\alpha}_{\mathbf{q}/2-\mathbf{k}'\downarrow} \hat{\alpha}_{\mathbf{q}/2+\mathbf{k}'\uparrow} \end{aligned} \quad (11)$$

Introducing the dressed wavefunction Eq. (4) is therefore equivalent to eliminating the bosonic degree of freedom from the theory by introducing effective purely fermionic quantities. We wish to point out that there is an alternative method of eliminating the bosonic degrees of freedom based on the application of the Hubbard-Stratonovich transformation to the functional integral expression for the partition function [16]. This is distinct from our approach, because it leads to a formal result in which the effective fermion-fermion interaction potential contains bare quantities, namely ν . In contrast the potential we give here is a real effective potential which contains only renormalized quantities, E or $\bar{\nu}$.

The implication of the above considerations goes beyond what we have presented so far, because the dressing procedure can be extended to treat correlation functions of any number of particles. It is now possible to make the direct link between the bare and the dressed correlation functions for a composite boson and a fermion pair, Eq. (3) and $f(\mathbf{r}_2, \mathbf{R})$. This can only be done assuming the contact scattering form for the boson-fermion vertex, i.e. that $g_{\mathbf{k}} = g$ independent of \mathbf{k} . Since this assumption leads to an ultraviolet divergent theory, we need to introduce a momentum cutoff K to the wavevector sums [11]. This implies for instance that the renormalized detuning in Eq. (6) is given by $\bar{\nu} = \nu - mKg^2/2\pi^2\hbar^2$. Recursively applying the same procedure used for the dressing of the two-fermion wavefunction, we are led to construct an ansatz for the four-fermion wavefunction:

$$\begin{aligned} \Psi_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}} &= \langle \hat{a}_{-\mathbf{q}/2-\mathbf{k}_1\downarrow} \hat{a}_{-\mathbf{q}/2+\mathbf{k}_1\uparrow} \hat{a}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle \\ &+ \beta_{\mathbf{k}_1} \langle \hat{b}_{-\mathbf{q}} \hat{a}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle \\ &+ \beta_{\mathbf{k}_2} \langle \hat{b}_{\mathbf{q}} \hat{a}_{-\mathbf{q}/2-\mathbf{k}_1\downarrow} \hat{a}_{-\mathbf{q}/2+\mathbf{k}_1\uparrow} \rangle \\ &- \beta_{(\mathbf{q}-\mathbf{k}_1-\mathbf{k}_2)/2} \langle \hat{b}_{\mathbf{k}_1-\mathbf{k}_2} \hat{a}_{-\mathbf{q}/2-\mathbf{k}_1\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle \\ &- \beta_{(\mathbf{q}+\mathbf{k}_1+\mathbf{k}_2)/2} \langle \hat{b}_{\mathbf{k}_2-\mathbf{k}_1} \hat{a}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{a}_{-\mathbf{q}/2+\mathbf{k}_1\uparrow} \rangle \\ &+ \beta_{\mathbf{k}_1} \beta_{\mathbf{k}_2} \langle \hat{b}_{-\mathbf{q}} \hat{b}_{\mathbf{q}} \rangle \\ &- \beta_{(\mathbf{q}-\mathbf{k}_1-\mathbf{k}_2)/2} \beta_{(\mathbf{q}+\mathbf{k}_1+\mathbf{k}_2)/2} \langle \hat{b}_{\mathbf{k}_2-\mathbf{k}_1} \hat{b}_{\mathbf{k}_1-\mathbf{k}_2} \rangle \end{aligned} \quad (12)$$

where $\beta_{\mathbf{k}} = \mathcal{P}\{g/(2\epsilon_{\mathbf{k}} - E)\}$. It can be shown that for four-particles in vacuum the evolution of this ansatz under the resonance Hamiltonian Eq. (2) is equivalent to the evolution of the four-particle wavefunction

$$\langle \hat{\alpha}_{-\mathbf{q}/2-\mathbf{k}_1\downarrow} \hat{\alpha}_{-\mathbf{q}/2+\mathbf{k}_1\uparrow} \hat{\alpha}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{\alpha}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle \quad (13)$$

under the single channel Hamiltonian Eq. (11), with the potential $U_{\mathbf{k},\mathbf{k}'}$ given in Eq. (8). Since we have proved that this interaction leads to the correct two-body T -matrix, this result is crucial because it is exactly the same equation which was solved in Ref. [5] to obtain the correct value of the boson-boson scattering length. It should also be clear that the procedure we have outlined can be systematically extended to incorporate more and more particles.

We are now in a position to make a definitive statement about the complete set of correlation functions in the resonance theory needed to reconstruct the information represented by $f(\mathbf{r}_2, \mathbf{R})$. Having two fermions approaching each other is equivalent to summing over one of the two relative momenta, e.g. \mathbf{k}_1 , in Eq. (13) or equivalently in Eq. (12). In this way we formulate the complete set:

$$\begin{aligned} &\langle \hat{b}_{-\mathbf{q}} \hat{b}_{\mathbf{q}} \rangle, \\ &\langle \hat{b}_{-\mathbf{q}} \hat{a}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle, \\ &\sum_{\mathbf{k}_1} \langle \hat{a}_{-\mathbf{q}/2-\mathbf{k}_1\downarrow} \hat{a}_{-\mathbf{q}/2+\mathbf{k}_1\uparrow} \hat{a}_{\mathbf{q}/2-\mathbf{k}_2\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}_2\uparrow} \rangle. \end{aligned} \quad (14)$$

The desired many-body theory must therefore include these correlation functions in order to generate the correct equation of state in the bosonic limit. We can now proceed to construct an approximate many-body theory using the standard methods of cumulant expansion [17] so that we keep explicitly the correlation functions in Eq. (14) and all the correlation functions of the same order. The key point is that the resulting theory closes within a set of functions which depend on a maximum of two vector arguments (e.g. the functions given in Eq. (14) depend at most on \mathbf{q} and \mathbf{k}_2). At a computational level, this is an essential point, because a two vector field in a translationally invariant system contains three nontrivial degrees of freedom, and a three dimensional theory is tractable. This is the minimal complexity because it is consistent with the intrinsic dimensionality of $f(\mathbf{r}_2, \mathbf{R})$ which encapsulates the few-body scattering calculation that this theory must reduce to in the limit of zero density. We also point out that this is an enormous simplification over the result of a direct application of the cumulant expansion to keep all correlation functions of order four fermions and below, i.e. including those of the form given in Eq. (13). Such a function depends on three vectors, and even in a uniform system, where rotational symmetries can be exploited, contains at least six nontrivial degrees of freedom.

It must be emphasized that the possibility of reducing the number of degrees of freedom in the whole crossover region is peculiar to the resonance Hamiltonian. This is because in order to close the set of equations in the many-body theory with three-particle correlation functions, it is crucial to apply the contact scattering approximation. In the resonance theory, Eq. (2), this implies $g_{\mathbf{k}} \rightarrow g$ independent of \mathbf{k} . However, the resulting effective potential Eq. (8) has a residual \mathbf{k} -dependence which makes the po-

tential and thus the theory well-defined even at $\bar{\nu} = 0$. However, in the single channel formulation, Eq. (11), this point causes problems as the scattering length $a_F \rightarrow \infty$ and the two-body T -matrix diverges. For this region there is no obvious way of incorporating correctly correlations of more than two particles in the many-body theory in a pseudopotential approximation. One can of course utilize a nonlocal potential and keep the full four-particle functions of the form in Eq. (13) in that case.

We now consider explicitly the consequence of the above formalism in the bosonic and fermionic superfluidity limits. The complete theory of the dilute nonideal Bose gas in the bosonic limit emerges naturally since it depends only on the eigensolution of the two-body problem and the interactions of the resulting dimers. Both of these elements we have discussed in depth. Thus, when the usual approximations are made, the Gross-Pitaevskii equation, the Bogoliubov theory, and the Popov theory, will emerge. In the fermionic limit, the set of correlation functions that we are keeping leads to the possibility of constructing a pair wavefunction that correctly includes the full many-body effects. In particular one can prove that the following ansatz:

$$\Psi_{\mathbf{k}} = \langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle - \sum_{\mathbf{q}} \beta_{\mathbf{q}/2+\mathbf{k}} \left(\langle \hat{b}_{\mathbf{q}} \hat{a}_{\mathbf{q}+\mathbf{k}\uparrow}^\dagger \hat{a}_{\mathbf{k}\uparrow} \rangle - \langle \hat{b}_{-\mathbf{q}} \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{-\mathbf{q}-\mathbf{k}\downarrow}^\dagger \rangle \right), \quad (15)$$

evolves using Eq. (2) as $\langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle$ evolves under the Hamiltonian in Eq. (11):

$$i\hbar \frac{d\langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle}{dt} = 2\epsilon_{\mathbf{k}} \langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{\mathbf{k}\uparrow} \rangle - \sum_{\mathbf{q}\mathbf{k}'} U_{\mathbf{q}/2+\mathbf{k},\mathbf{k}'} \left(\langle \hat{a}_{\mathbf{q}+\mathbf{k}\uparrow}^\dagger \hat{a}_{\mathbf{k}\uparrow} \hat{a}_{\mathbf{q}/2-\mathbf{k}'\downarrow} \hat{a}_{\mathbf{q}/2+\mathbf{k}'\uparrow} \rangle - \langle \hat{a}_{-\mathbf{k}\downarrow} \hat{a}_{-\mathbf{q}-\mathbf{k}\downarrow}^\dagger \hat{a}_{-\mathbf{q}/2-\mathbf{k}'\downarrow} \hat{a}_{-\mathbf{q}/2+\mathbf{k}'\uparrow} \rangle \right). \quad (16)$$

Eq. (16) shows that Eq. (15) contains the full pair wavefunction in the medium and not just the BCS approximate factorized form. Notice that an analogous ansatz and correspondence can be formulated for the density correlation function $\langle \hat{a}_{\mathbf{k}\uparrow}^\dagger \hat{a}_{\mathbf{k}\uparrow} \rangle$. Together these imply that we not only recover the complete BCS equations but also the effects beyond mean-field such as the Gorkov corrections to the superfluid gap.

In conclusion, a consistent theoretical framework has been presented for the crossover of superfluidity from the fermionic to the bosonic type. The inclusion of the correlation function between a boson and a fermion pair was required to reproduce the correct bosonic equation of state. This has lead us to develop a fundamental change to the picture of the crossover physics.

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